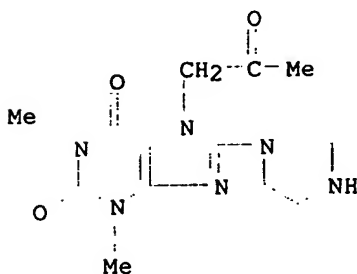
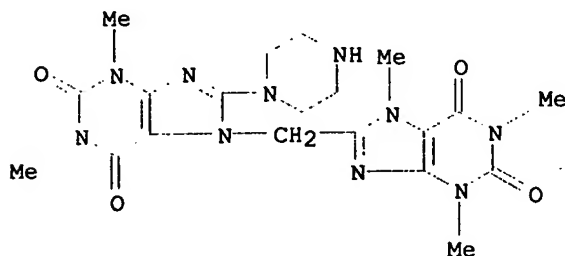


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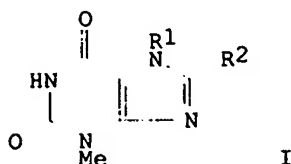
AN 1969:459503 CAPLUS
 DN 71:59503
 TI Pharmacological studies of basic theophylline derivatives. I. Effects on the cardiovascular system
 AU Kubota, Kazuhiko; Kono, Shigeharu; Koreeda, Tadako
 CS Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, Japan
 SO Yakugaku Zasshi (1969), 89(4), 441-5
 CODEN: YKKZAJ
 DT Journal
 LA Japanese
 CC 15 (Pharmacodynamics)
 GI For diagram(s), see printed CA Issue.
 AB The following new theophylline (I) derivs. were evaluated for their cardiovascular effects on dogs (7- and 8-substituents and m.p. given): CH₂CH₂C(:NOH)NH₂, H, 203-5.degree.; CH₂C(:NOH)NH₂, H, 227-30.degree.; CH₂Ac, piperazino, 192.degree.; CH₂Ac, morpholino, 167.degree.. Also tested were II (R, R1, and m.p. given): Bu, H, 93.degree.; Et, Et, 85.degree.; (RR1 =) piperidino, 158.degree.; (RR1 =) morpholino, 178.degree.; (RR1 =) pyrrolidino, 112.degree.; and III (R2 and m.p. given): piperidino, 202.degree.; Et₂N, 160.degree. (IV). Most of the compds. increased the blood flow of renal, femoral, and internal carotid arteries, but the effect was of the order of that of I. IV, however, was 6-fold as effective in the internal carotid blood flow. In general, addn. of basic polar groups to I lessened the cardiovascular effects.
 ST theophyllines blood flow; blood flow theophyllines; cardiovascular drugs
 IT Circulation
 Heart
 (theophylline derivs. effect on)
 IT 22270-11-7 22270-12-8 22275-47-4 22275-48-5 22275-50-9
 22285-89-8 24961-80-6 24961-81-7 24961-83-9 24961-85-1
 24961-86-2
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (pharmacology of)
 IT 24961-80-6
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (pharmacology of)
 RN 24961-80-6 CAPLUS
 CN Theophylline, 7-acetonyl-8-(1-piperazinyl)- (8CI) (CA INDEX NAME)



AN 1970:55410 CAPLUS
 DN 72:55410
 TI Synthesis of substituted bisxanthines
 AU Kleine, K. H.; Graefe, Guenter; Haller, Rolf
 CS Pharm. Inst., Univ. Freiburg/Br., Freiburg/Br., Ger.
 SO Arzneim.-Forsch. (1969), 19(11), 1854-5
 CODEN: ARZNAD
 DT Journal
 LA German
 CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))
 GI For diagram(s), see printed CA Issue.
 AB I (R = Br) (3.3 millimoles) was treated with 33 millimoles piperidine in 15 ml EtOH 13 hr at 140-5.degree. to give 72% I (R = piperidino), m. 176-8.degree.. The following compds. were similarly prepd. (compd., R, % yield, and m.p. given): I, morpholino, 75, 208-10.degree.; I, NEt₂, 86, 130-1.degree.; I, iso-PrNH, 88, 188-90.degree.; I, NHCH₂CH₂OH, 96, 219-21.degree.; II, piperidino, 99, 265-6.degree. (decompn.); II, 1-piperazinyl, 100, 250-2.degree. (decompn.); II, 4-(2-hydroxyethyl)-1-piperazinyl, 94, 279-80.degree.. I (R = Br) (4 g) was refluxed with 4.53 g NaSH in 120 ml 80% iso-PrOH 2 hr to give 69% I (R = SH), m. 190-2.degree. (decompn.), which on treatment with NaOAc-MeI gave 82% I (R = SMe), m. 258-9.degree.. I (R = SEt), m. 188-9.degree. (decompn.), was similarly prepd. in 72% yield.
 ST bisxanthines synthesis
 IT 25472-84-8P 25472-85-9P 25472-86-0P 25472-87-1P 25472-88-2P
 25472-89-3P 25472-90-6P 25472-91-7P 25472-92-8P 25472-93-9P
 25472-94-0P 25583-99-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 IT 25472-93-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 25472-93-9 CAPLUS
 CN Caffeine, 8-[[1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-8-(1-piperazinyl)purin-7-yl]methyl]- (8CI) (CA INDEX NAME)



AN 1987:95577 CAPLUS
 DN 106:95577
 TI Synthesis and biological activity of 3-methyl, 7- or 8-alkyl-,
 7,8-dialkyl, heterocyclic, and cyclohexylaminoxanthines
 AU Romanenko, N. I.; Fedulova, I. V.; Primenko, B. O.; Orestenko, L. P.
 CS Zaporozh. Med. Inst., Zaporozhe, USSR
 SO Farm. Zh. (Kiev) (1986), (5), 41-4
 CODEN: FRZKAP; ISSN: 0367-3057
 DT Journal
 LA Ukrainian
 CC 1-3 (Pharmacology)
 Section cross-reference(s): 28
 GI



AB Seventeen title compds. (I; R1 = heptyl, nonyl, or CH₂CH:C(Cl)Me; R2 = NMe₂, NEt₂, piperidino, cyclohexylamino, NHCH₂Ph, piperazino, morpholino, NHHN₂, N(CH₂CH₂OH)₂, etc.) were prepd. by reacting the K salt of 8-bromo-3-methylxanthine with appropriate alkyl halides followed by condensation with appropriate primary or secondary amines. Toxicity studies in mice showed I to be less toxic than aminazine. Most I exhibited diuretic activity in rats, and some exhibited analeptic activity as well. Many I exhibited antimicrobial activity in vitro against both bacteria and fungi. The most active diuretics contained morpholino, piperidino, or N-benzyl groups at the 8-position.

ST methylxanthine deriv prepn pharmacol; diuretic methylxanthine deriv prepn; structure activity xanthine deriv prepn; alkylaminoxanthine prepn pharmacol

IT Bactericides, Disinfectants, and Antiseptics
 (alkylaminoxanthines as)

IT Diuretics
 (alkylaminoxanthines as, structure in relation to)

IT Toxicity
 (of alkylaminoxanthines)

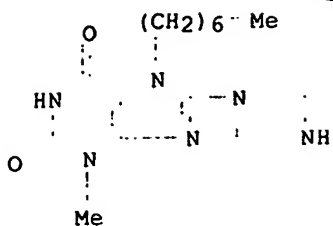
IT Molecular structure-biological activity relationship
 (diuretic, of alkylaminoxanthines)

IT 1076-22-8DP, derivs. 106939-13-3P 106939-14-4P 106939-15-5P
 106939-16-6P 106939-17-7P 106939-18-8P 106939-19-9P 106939-20-2P
 106939-21-3P 106939-22-4P 106939-23-5P 106939-24-6P
 106939-25-7P 106939-26-8P 106939-27-9P 106939-28-0P
 106939-29-1P 106960-61-6P 106960-62-7P 106960-63-8P
 RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
 (prepn. and pharmacol. of, structure in relation to)

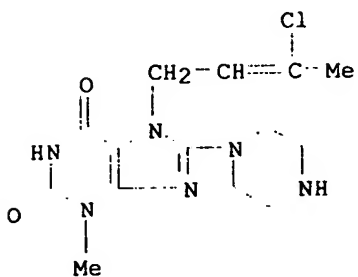
IT 106939-21-3P 106939-29-1P
 RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
 (prepn. and pharmacol. of, structure in relation to)

RN 106939-21-3 CAPLUS

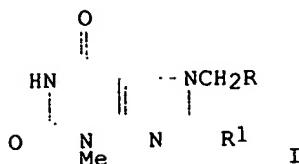
CN 1H-Purine-2,6-dione, 7-heptyl-3,7-dihydro-3-methyl-8-(1-piperazinyl)-
 (9CI) (CA INDEX NAME)



RN 106939-29-1 CAPLUS
 CN 1H-Purine-2,6-dione, 7-(3-chloro-2-butenyl)-3,7-dihydro-3-methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)



AN 1986:626150 CAPUS
 DN 105:226150
 TI Synthesis, neurotropic and diuretic activity of 7,8-disubstituted
 3-methylxanthines
 AU Samura, B. A.; Fedulova, I. V.; Romanenko, B. A.; Priimenko, B. A.;
 Chervinskii, A. Yu.; Garmash, S. N.; Troshin, D. A.
 CS Zaporozh. Med. Inst., Zaporozh, USSR
 SO Khim.-Farm. Zh. (1986), 20(1), 52-5
 CODEN: KHFZAN; ISSN: 0023-1134
 DT Journal
 LA Russian
 CC 26-9 (Biomolecules and Their Synthetic Analogs)
 Section cross-reference(s): 1, 28
 OS CASREACT 105:226150
 GI



AB The title compds. I (R = Ph, CH₂OPh, CH(OH)C₆H₄NO₂-p, R₁ =
 2-furylmethylamino, morpholino, hexamethylenimino, NHCH₂CH₂OH, NEt₂,
 piperazino, SCH₂CO₂H), useful as psychotropics and diuretics, were prepd.
 in 24-94% yields from I (R₁ = Br) by amination with appropriate amines or
 by reaction with HSCH₂CO₂H. The hydrochloride of I [R = CH(OH)C₆H₄NO₂-p,
 R₁ = piperazino] increased urinary flow 180.7% compared to a control and
 potentiated narcotic sleep 147.0% compared to a control.

ST xanthine amino psychotropic diuretic
 IT Diuretics
 Psychotropics
 (disubstituted methylxanthines)

IT 93703-25-4
 RL: RCT (Reactant)
 (alkylation of)

IT 68-11-1, reactions 104-63-2 109-89-7, reactions 110-85-0, reactions
 110-91-8, reactions 111-49-9 141-43-5, reactions 617-89-0
 RL: RCT (Reactant)
 (amination by, of bromomethylxanthines)

IT 93703-26-5P 93703-27-6P 101072-18-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn., amination, and reaction with thioglycolic acid)

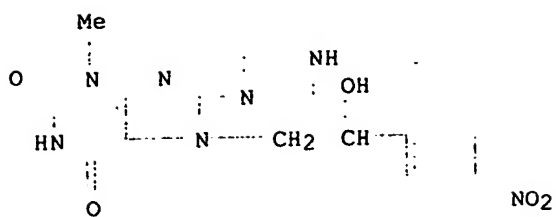
IT 105522-54-1P 105522-55-2P 105522-56-3P 105522-57-4P 105522-58-5P
 105522-59-6P 105522-60-9P 105522-61-0P 105522-62-1P
 105522-63-2P 105522-64-3P 105522-65-4P 105522-66-5P 105522-67-6P
 105522-68-7P 105522-69-8P 105522-70-1P 105522-71-2P 105522-72-3P
 105522-73-4P 105522-74-5P 105522-75-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn., psychotropic, and diuretic activity of)

IT 105522-76-7 105522-77-8 105542-90-3
 RL: RCT (Reactant)
 (reaction of, with bromobenzylmethylcaffeine)

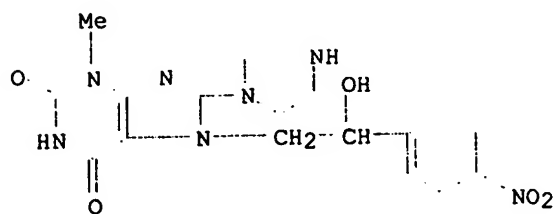
IT 6388-74-5
 RL: RCT (Reactant)
 (reaction of, with methylbromoxanthene potassium salt)

IT 105522-61-0P 105522-62-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn., psychotropic, and diuretic activity of)

RN 105522-61-0 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-2-(4-nitrophenyl)ethyl]-3-
 methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)

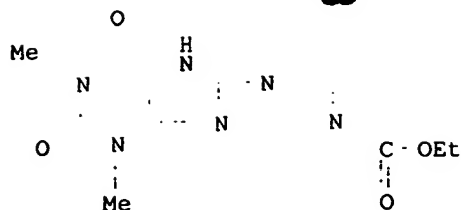


RN 105522-62-1 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-2-(4-nitrophenyl)ethyl]-3-methyl-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

AN 1975:80351 CAPLUS
 DN 82:80351
 TI Piperazine derivatives of methylxanthines. I. Chemical and pharmacological properties of 8-piperazinotheophyllines
 AU Górczyca, M.; Zejč, A.; Krupinska, J.; Czarnecki, R.
 CS Dep. Pharm. Chem., Med. Acad. Cracow, Krakow, Pol.
 SO Farmaco, Ed. Sci. (1974), 29(10), 802-10
 CODEN: FRPSAX
 DT Journal
 LA English
 CC 1-3 (Pharmacodynamics)
 GI For diagram(s), see printed CA Issue.
 AB 8-Bromotheophylline [10357-68-3] was heated with the appropriate piperazines to yield 8-piperazinotheophylline (I) [54119-57-2], N-(8-theophyllinyl)-N'-methylpiperazine [52943-65-4], N-(8-theophyllinyl)-N'-.beta.-hydroxyethylpiperazine [40171-75-3], and N-(8-theophyllinyl)-N'-benzylpiperazine [54119-58-3]. I had a strong antihistaminic action on guinea pig trachea and a weak one on guinea pig and rat ileum. Tests on exptl. animals showed that the acute toxicities of these compds. were lower than those of aminophylline [317-34-0] and theophylline Na acetate [8002-89-9], and their hypotensive and cardiac actions were weaker than those of aminophylline.
 ST methylxanthine heart action; antihistamine piperazinotheophylline; theophylline blood pressure
 IT Molecular structure-biological activity relationship
 (antihistaminic, of piperazinotheophyllines)
 IT Antihistaminics
 (piperazinotheophyllines)
 IT Heart
 (piperazinotheophyllines effect on)
 IT Hypotension
 (piperazinotheophyllines in relation to)
 IT 317-34-0 8002-89-9
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (pharmacology of, piperazinotheophyllines in relation to)
 IT 54119-63-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and hydrolysis of)
 IT 40171-75-3P 52943-65-4P 54119-57-2P 54119-58-3P
 RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
 (prepn. and pharmacol. of)
 IT 54119-59-4P 54119-60-7P 54119-61-8P 54119-62-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 IT 120-43-4
 RL: RCT (Reactant)
 (reaction of, with bromotheophylline)
 IT 10357-68-3
 RL: RCT (Reactant)
 (reaction of, with piperazine derivatives)
 IT 110-85-0, reactions
 RL: RCT (Reactant)
 (with bromotheophylline)
 IT 54119-63-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and hydrolysis of)
 RN 54119-63-0 CAPLUS
 CN 1-Piperazinecarboxylic acid, 4-(2,3,6,7-tetrahydro-1,3-dimethyl-2,6-dioxo-1H-purin-8-yl)-, ethyl ester (9CI) (CA INDEX NAME)

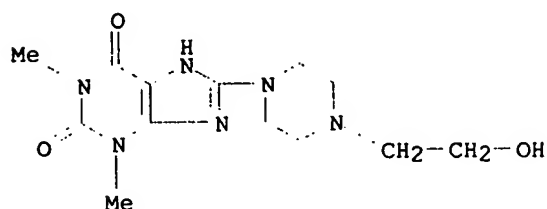


IT 40171-75-3P 52943-65-4P 54119-57-2P
54119-58-3P

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses) (prepn. and pharmacol. of)

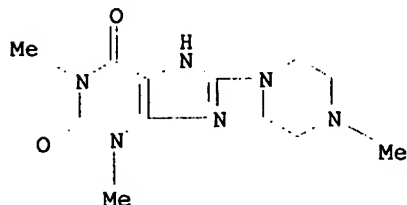
RN 40171-75-3 CAPLUS

CN 1H-Purine-2,6-dione, 3,7-dihydro-8-[(4-(2-hydroxyethyl)-1-piperazinyl)-1,3-dimethyl- (9CI)] (CA INDEX NAME)



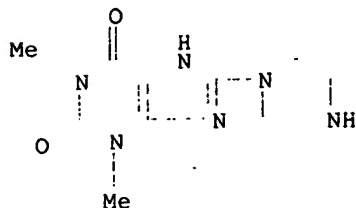
RN 52943-65-4 CAPLUS

CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



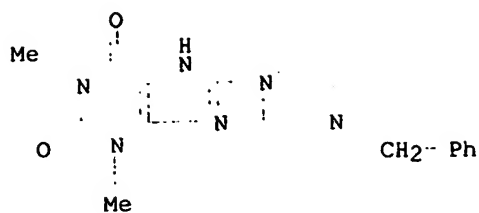
RN 54119-57-2 CAPLUS

CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)



RN 54119-58-3 CAPLUS

CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-[(4-(phenylmethyl)-1-piperazinyl)- (9CI)] (CA INDEX NAME)



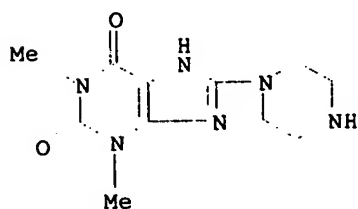
IT 54119-59-4P 54119-60-7P 54119-61-8P

54119-62-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 54119-59-4 CAPLUS

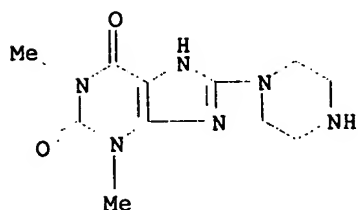
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(1-piperazinyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 54119-60-7 CAPLUS

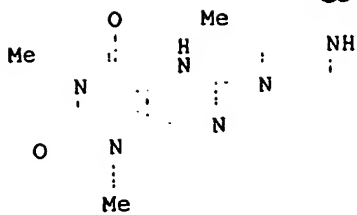
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(1-piperazinyl)-,
monohydrobromide (9CI) (CA INDEX NAME)



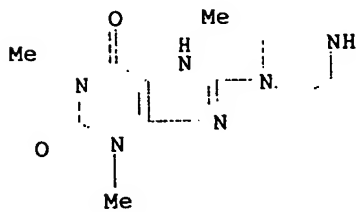
● HBr

RN 54119-61-8 CAPLUS

CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(2-methyl-1-piperazinyl)-
(9CI) (CA INDEX NAME)



RN 54119-62-9 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(2-methyl-1-piperazinyl)-,
 monohydrochloride (9CI) (CA INDEX NAME)



● HCl

AN 1999:559580 CAPLUS
 DN 131:351159
 TI Synthesis of 8-substituted xanthenes and their oxidative skeleton
 rearrangement to 1-oxo-2,4,7,9-tetraazaspiro[4,5]dec-2-ene-6,8,10-triones
 AU Zimmer, Hans; Amer, Adel; Baumann, Frank M.; Haecker, Michael; Hess,
 Christopher G. M.; Ho, Douglas; Huber, Hans J.; Koch, Klaus; Mahnke, K.;
 Schumacher, Christian; Wingfield, Robert C.
 CS Dep. Chemistry, Univ. Cincinnati, Cincinnati, OH, 45221, USA
 SO Eur. J. Org. Chem. (1999), (9), 2419-2428
 CODEN: EJOCFK; ISSN: 1434-193X
 PB Wiley-VCH Verlag GmbH
 DT Journal
 LA English
 CC 26-9 (Biomolecules and Their Synthetic Analogs)
 OS CASREACT 131:351159
 AB The synthesis of a no. of 8-(dialkylamino)xanthenes- and 8-alkoxyxanthenes
 is described. Treatment of 8-(dialkylamino)xanthenes with 3-ClC6H4CO3H
 (m-CPBA) gave 3-(dialkylamino)-4,7,9-trimethyl-1-oxo-2,4,7,9-
 tetraazaspiro[4,5]dec-2-ene-6,8,10-triones by a novel rearrangement.
 Also, the corresponding 3-alkoxylated spiro compds. were obtained by an
 analogous treatment of 8-alkoxyxanthenes. In attempts to elucidate a
 tentative mechanism for this rearrangement, 8-
 [(dialkylamino)methyl]caffeines on treatment with m-CPBA did not undergo
 the rearrangement but only yielded the expected N-oxides. This result
 seems to indicate that a necessary structure element for this
 rearrangement to occur is an atom with an unshared pair of electrons to be
 attached to the 8-position of the investigated xanthenes. In agreement
 with this statement is the fact that N-oxides of 8-
 [(dialkylamino)methyl]caffeines do not undergo the novel rearrangement but
 rather give the expected Meisenheimer rearrangement or the Cope
 elimination depending upon reaction conditions.
 ST tetraazaspirodecenetrione prepn; xanthine prepn oxidative rearrangement
 IT Rearrangement
 (oxidative; of xanthenes to tetraazaspiro[4,5]decenetriones)
 IT Purine bases
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of xanthenes and oxidative rearrangement to
 tetraazaspiro[4,5]decenetriones)
 IT Oxidation
 (rearrangement; of xanthenes to tetraazaspiro[4,5]decenetriones)
 IT 129315-74-8P 250648-49-8P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (crystal structure)
 IT 4921-50-0P
 RL: BYP (Byproduct); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of xanthenes and oxidative rearrangement to
 tetraazaspiro[4,5]decenetriones)
 IT 62-53-3, Benzenamine, reactions 75-89-8, 2,2,2-Trifluoroethanol
 100-61-8, N-Methylaniline, reactions 109-05-7, 2-Methylpiperidine
 110-85-0, Piperazine, reactions 110-91-8, Morpholine, reactions
 110-96-3, Diisobutylamine 142-25-6, N,N,N'-Trimethyl-1,2-ethanediamine
 544-00-3, Diisopentylamine 569-34-6 577-66-2 2050-92-2,
 Dipentylamine 2099-74-3 4543-96-8, N,N,N'-Trimethyl-1,3-propanediamine
 5436-38-4 5436-39-5 6326-68-7 10381-82-5 71411-94-4 78146-62-0
 130216-53-4 130332-80-8 146787-63-5, Butyl proline 250648-34-1
 250648-35-2 250648-50-1 250648-51-2
 RL: RCT (Reactant)
 (prepn. of xanthenes and oxidative rearrangement to
 tetraazaspiro[4,5]decenetriones)
 IT 6743-03-9P 6968-57-6P 50693-74-8P 135101-47-2P
 157063-97-3P 250648-36-3P 250648-37-4P 250648-38-5P 250648-39-6P
 250648-40-9P 250648-41-0P 250648-42-1P 250648-44-3P 250648-45-4P
 250648-55-6P 250648-56-7P 250648-57-8P 250648-58-9P 250648-75-0P
 250648-76-1P 250648-77-2P 250648-79-4P 250648-80-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of xanthenes and oxidative rearrangement to
 tetraazaspiro[4,5]decenetriones)
 IT 129315-68-0P 129315-69-1P 129315-70-4P 129315-71-5P 129315-72-6P

129315-73-7P	157063-93-9P	250648-43-2P	250648-46-5P	
250648-47-6P	250648-48-7P	250648-52-3P	250648-53-4P	250648-54-5P
250648-59-0P	250648-60-3P	250648-61-4P	250648-62-5P	250648-63-6P
250648-64-7P	250648-65-8P	250648-66-9P	250648-67-0P	250648-68-1P
250648-69-2P	250648-70-5P	250648-71-6P	250648-72-7P	250648-73-8P
250648-74-9P	250648-81-8P	250648-82-9P	250648-83-0P	250648-84-1P
250648-85-2P				

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of xanthines and oxidative rearrangement to
tetraazaspiro[4,5]decenetriones)

RE.CNT 34

RE

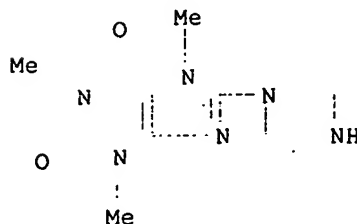
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- (34) Zimmer, H; J Org Chem 1990, V55, P4988 CAPLUS

IT 50693-74-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of xanthines and oxidative rearrangement to
tetraazaspiro[4,5]decenetriones)

RN 50693-74-8 CAPLUS

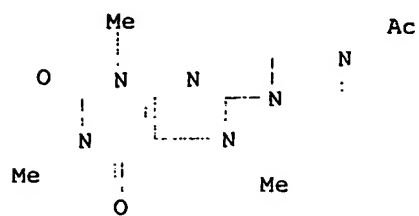
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-8-(1-piperazinyl)- (9CI)
(CA INDEX NAME)



IT 250648-43-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of xanthines and oxidative rearrangement to
tetraazaspiro[4,5]decenetriones)
RN 250648-43-2 CAPLUS
CN Piperazine, 1-acetyl-4-(2,3,6,7-tetrahydro-1,3,7-trimethyl-2,6-dioxo-1H-
purin-8-yl)- (9CI) (CA INDEX NAME)



AN 1977:139992 CAPLUS
 DN 86:139992
 TI 1,8-Disubstituted derivatives of theobromine and their pharmacological activity
 AU Gutorov, L. A.; Ovcharova, I. M.; Golovchinskaya, E. S.; Muratov, M. A.; Kaminka, M. E.; Mashkovskii, M. D.
 CS Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR
 SO Khim.-Farm. Zh. (1976), 10(12), 61-4
 CODEN: KHFZAN
 DT Journal
 LA Russian
 CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 1
 GI



AB Theobromine derivs. I (R = II, R1 = Et2NCH2) were obtained in 68.5 and 71.7% yields by heating I (R = H) with chloroalkyl 3,4,5-trimethoxybenzoates. Analogous alkylation of I (R = H, R1 = Cl) gave 70.4 and 42.2% I (R = II, R1 = Cl) which were aminated by piperazine derivs. to give 78.2-84.5% I (R = II, R1 = 1-piperazinyl, 4-methyl-1-piperazinyl). Alkylation of the latter with Cl(CH2)nOH (n = 2,3), and ClCH2CH(OH)CH2OH gave 40.5-70.4% of the hydroxyalkylpiperazinyl theobromine derivs. I were useful as broncholytics, vasodilators, and as antihypertensives.

ST theobromine broncholytic prepn; vasodilator theobromine prepn; antihypertensive theobromine prepn

IT Vasodilators
 (by disubstituted theobromine derivs.)

IT Bronchodilators
 (disubstituted theobromine derivs.)

IT Antihypertensives
 (disubstituted theobromine derivs. in treatment of)

IT 4921-55-5 15996-30-2
 RL: RCT (Reactant)
 (alkylation of)

IT 1027-24-3 1029-24-9
 RL: RCT (Reactant)
 (alkylation of theobromine derivs. by)

IT 109-01-3 110-85-0, reactions
 RL: RCT (Reactant)
 (amination of chlorotheobromine derivs. by)

IT 62128-66-9P 62128-67-0P 62128-68-1P 62128-69-2P
 62128-70-5P 62128-71-6P 62128-72-7P
 62128-75-0P 62128-76-1P 62128-77-2P
 62164-83-4P 62164-84-5P
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (prepn. and pharmacol. activity of)

IT 62128-73-8P 62128-74-9P 62128-78-3P 62128-79-4P
 62128-80-7P 62128-81-8P 62128-82-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

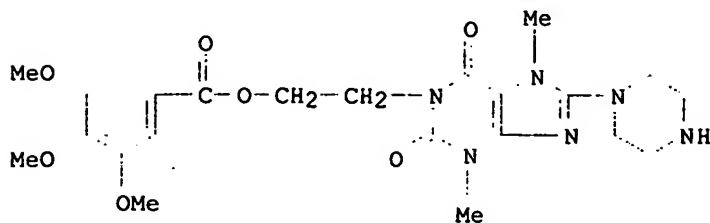
IT 96-24-2 107-07-3, reactions 627-30-5
 RL: RCT (Reactant)
 (reaction of, with piperazinyltheobromine derivs.)

IT 62128-69-2P 62128-70-5P 62128-71-6P
 62128-72-7P 62128-75-0P 62128-76-1P
 62128-77-2P 62164-84-5P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and pharmacol. activity of)

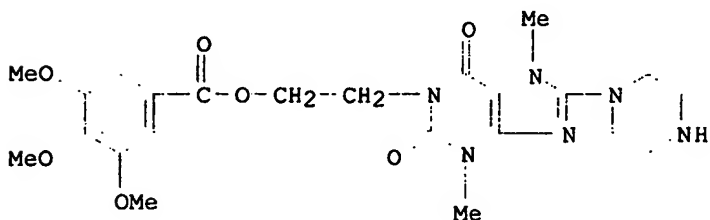
RN 62128-69-2 CAPLUS

CN Benzoic acid, 3,4,5-trimethoxy-, 2-[2,3,6,7-tetrahydro-3,7-dimethyl-2,6-dioxo-8-(1-piperazinyl)-1H-purin-1-yl]ethyl ester (9CI) (CA INDEX NAME)



RN 62128-70-5 CAPLUS

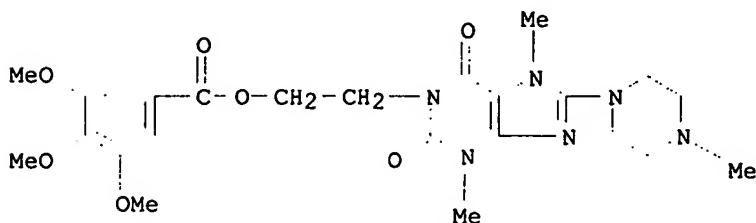
CN Benzoic acid, 3,4,5-trimethoxy-, 2-[2,3,6,7-tetrahydro-3,7-dimethyl-2,6-dioxo-8-(1-piperazinyl)-1H-purin-1-yl]ethyl ester, monohydrochloride (9CI)
(CA INDEX NAME)



● HCl

RN 62128-71-6 CAPLUS

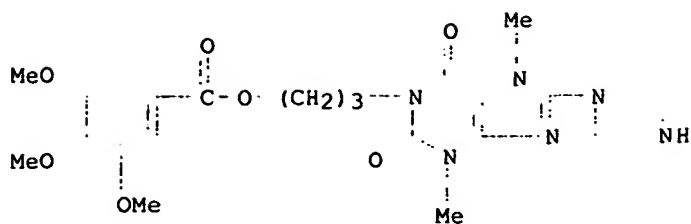
CN Benzoic acid, 3,4,5-trimethoxy-, 2-[2,3,6,7-tetrahydro-3,7-dimethyl-8-(4-methyl-1-piperazinyl)-2,6-dioxo-1H-purin-1-yl]ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



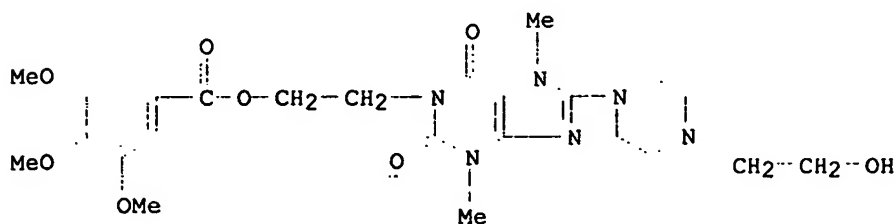
● HCl

RN 62128-72-7 CAPLUS

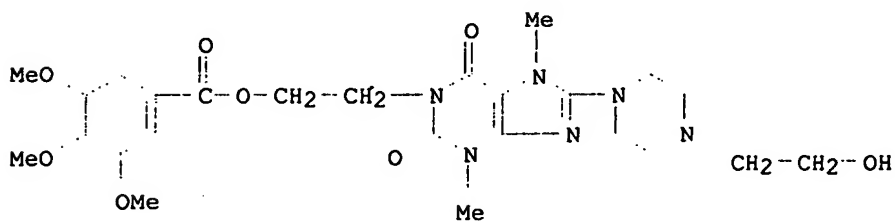
CN Benzoic acid, 3,4,5-trimethoxy-, 3-[2,3,6,7-tetrahydro-3,7-dimethyl-2,6-dioxo-8-(1-piperazinyl)-1H-purin-1-yl]propyl ester (9CI) (CA INDEX NAME)



RN 62128-75-0 CAPLUS
 CN Benzoic acid, 3,4,5-trimethoxy-, 2-[2,3,6,7-tetrahydro-8-[4-(2-hydroxyethyl)-1-piperazinyl]-3,7-dimethyl-2,6-dioxo-1H-purin-1-yl]ethyl ester (9CI) (CA INDEX NAME)

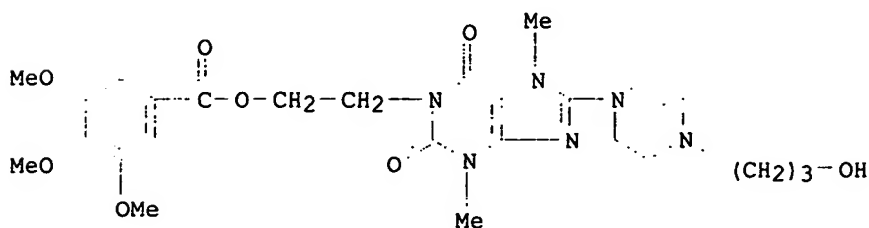


RN 62128-76-1 CAPLUS
 CN Benzoic acid, 3,4,5-trimethoxy-, 2-[2,3,6,7-tetrahydro-8-[4-(2-hydroxyethyl)-1-piperazinyl]-3,7-dimethyl-2,6-dioxo-1H-purin-1-yl]ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



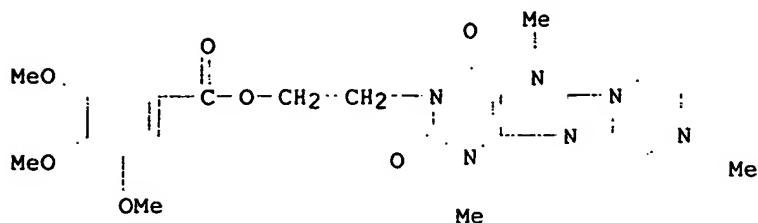
● HCl

RN 62128-77-2 CAPLUS
 CN Benzoic acid, 3,4,5-trimethoxy-, 2-[2,3,6,7-tetrahydro-8-[4-(3-hydroxypropyl)-1-piperazinyl]-3,7-dimethyl-2,6-dioxo-1H-purin-1-yl]ethyl ester (9CI) (CA INDEX NAME)



RN 62164-84-5 CAPLUS
 CN Benzoic acid, 3,4,5-trimethoxy-, 2-[2,3,6,7-tetrahydro-3,7-dimethyl-8-(4-

methyl-1-piperazinyl)-2,6-dioxo-1H-purin-1-yl]ethyl ester (9CI) (CA INDEX NAME)

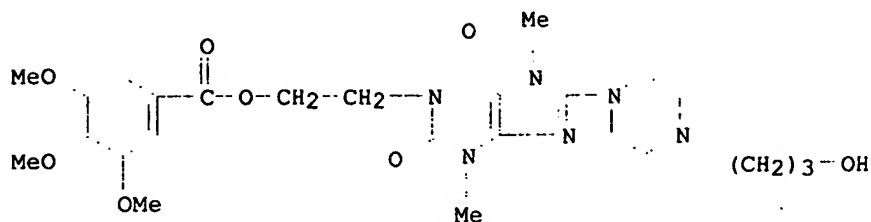


IT 62128-78-3P 62128-79-4P 62128-80-7P
62128-81-8P 62128-82-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 62128-78-3 CAPLUS

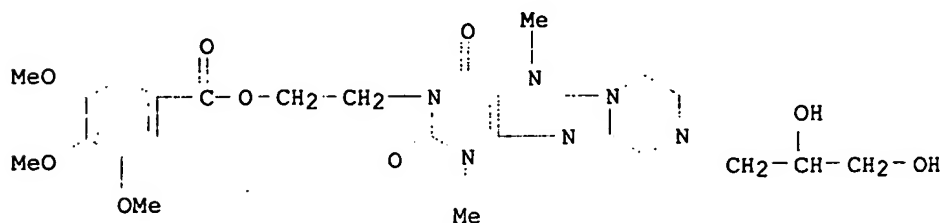
CN Benzoic acid, 3,4,5-trimethoxy-, 2-[2,3,6,7-tetrahydro-8-[4-(3-hydroxypropyl)-1-piperazinyl]-3,7-dimethyl-2,6-dioxo-1H-purin-1-yl]ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

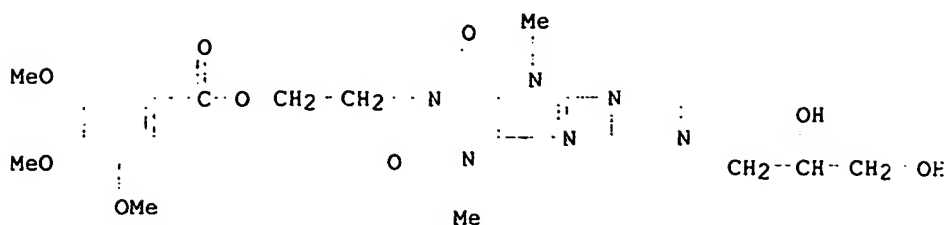
RN 62128-79-4 CAPLUS

CN Benzoic acid, 3,4,5-trimethoxy-, 2-[8-[4-(2,3-dihydroxypropyl)-1-piperazinyl]-2,3,6,7-tetrahydro-3,7-dimethyl-2,6-dioxo-1H-purin-1-yl]ethyl ester (9CI) (CA INDEX NAME)



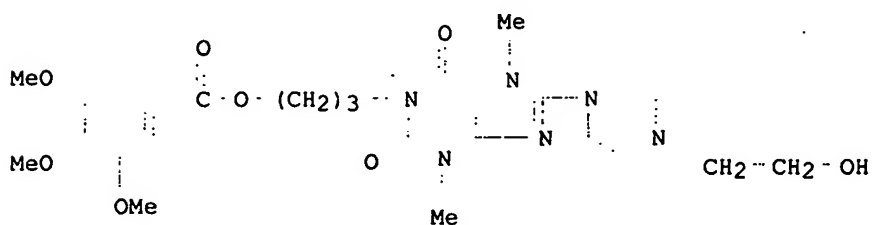
RN 62128-80-7 CAPLUS

CN Benzoic acid, 3,4,5-trimethoxy-, 2-[8-[4-(2,3-dihydroxypropyl)-1-piperazinyl]-2,3,6,7-tetrahydro-3,7-dimethyl-2,6-dioxo-1H-purin-1-yl]ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

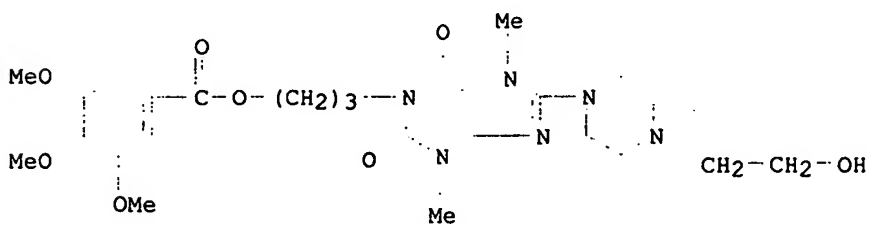


● HCl

RN 62128-81-8 CAPLUS
 CN Benzoic acid, 3,4,5-trimethoxy-, 3-[2,3,6,7-tetrahydro-8-[4-(2-hydroxyethyl)-1-piperazinyl]-3,7-dimethyl-2,6-dioxo-1H-purin-1-yl]propyl ester (9CI) (CA INDEX NAME)

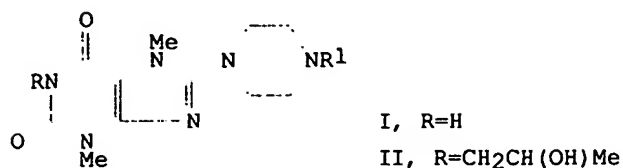


RN 62128-82-9 CAPLUS
 CN Benzoic acid, 3,4,5-trimethoxy-, 3-[2,3,6,7-tetrahydro-8-[4-(2-hydroxyethyl)-1-piperazinyl]-3,7-dimethyl-2,6-dioxo-1H-purin-1-yl]propyl ester, monohydrochloride (9CI) (CA INDEX NAME)

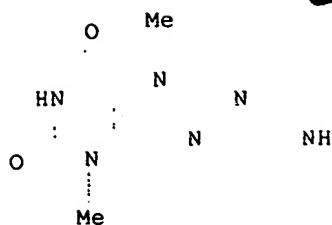


● HCl

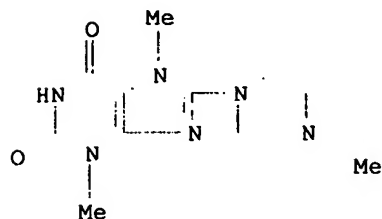
AN 1978:509376 CAPLUS
 DN 89:109376
 TI Piperazine derivatives of dimethylxanthines. V. Preparation and properties of 8-piperazino- and 1-.beta.-hydroxypropyl-8-piperazinotheobromines
 AU Cygankiewicz, Andrzej; Gorczyca, Maria; Zejc, Alfred; Zimon, Romuald
 CS Dep. Pharm. Chem., Sch. Med., Krakow, Pol.
 SO Acta Pol. Pharm. (1977), 34(6), 607-12
 CODEN: APPHAX; ISSN: 0001-6837
 DT Journal
 LA Polish
 CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
 GI



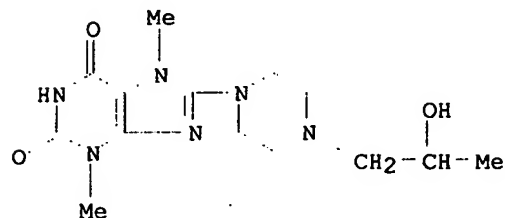
AB 8-Bromotheobromine and anhyd. piperazine heated in MeOCH₂CH₂OH gave 67% I (R₁ = H). I [R₁ = Me, CH₂CH₂OH, and CH₂CH(OH)Me] were prepd. analogously in 68-72% yields. I heated in PrOH with 2,3-epoxypropane in presence of pyridine gave 48-75% II [R₁ = H, Me, CH₂CH(OH)Me], which were also obtained in the reaction of 1-(.beta.-hydroxypropyl)-8-bromotheobromine with the appropriately substituted piperazine. All I and II were characterized as HCl or HBr salts, and most of the hydroxylated I and II, also as the Ac derivs. I and II were synthesized as potential spasmolytics and antihistaminics.
 ST theobromine piperazino hydroxypropyl; spasmolytic piperazinotheobromine; antihistaminic piperazinotheobromine
 IT Anticonvulsants and Antiepileptics
 Antihistaminics
 (potential, piperazinotheobromines)
 IT 67162-64-5P 67162-66-7P 67162-71-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and reaction with propylene oxide)
 IT 67162-65-6P 67162-67-8P 67162-68-9P
 67162-69-0P 67162-70-3P 67162-72-5P
 67162-73-6P 67162-74-7P 67162-75-8P
 67162-76-9P 67162-77-0P 67162-78-1P
 67162-79-2P 67162-80-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 IT 103-76-4 109-01-3 110-85-0, reactions 1074-54-0
 RL: RCT (Reactant)
 (reaction of, with bromotheobromine)
 IT 15371-15-0
 RL: RCT (Reactant)
 (reaction of, with piperazine)
 IT 957-47-1
 RL: RCT (Reactant)
 (reaction of, with piperazines)
 IT 67162-64-5P 67162-66-7P 67162-71-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and reaction with propylene oxide)
 RN 67162-64-5 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl-8-(1-piperazinyl)- (9CI)
 (CA INDEX NAME)



RN 67162-66-7 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl-8-(4-methyl-1-piperazinyl)-
 (9CI) (CA INDEX NAME)

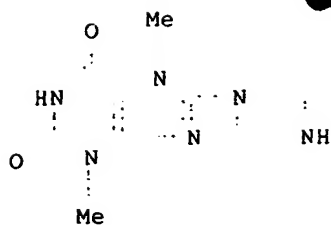


RN 67162-71-4 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-8-[4-(2-hydroxypropyl)-1-piperazinyl]-3,7-
 dimethyl- (9CI) (CA INDEX NAME)



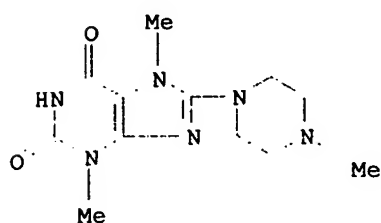
IT 67162-65-6P 67162-67-8P 67162-68-9P
 67162-69-0P 67162-70-3P 67162-72-5P
 67162-73-6P 67162-74-7P 67162-75-8P
 67162-76-9P 67162-77-0P 67162-78-1P
 67162-79-2P 67162-80-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 67162-65-6 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl-8-(1-piperazinyl)-,
 dihydrochloride (9CI) (CA INDEX NAME)



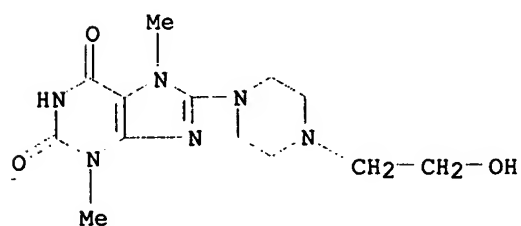
● 2 HCl

RN 67162-67-8 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl-8-(4-methyl-1-piperazinyl)-, monohydrobromide (9CI) (CA INDEX NAME)

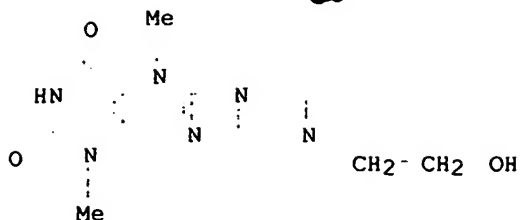


● HBr

RN 67162-68-9 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-8-[4-(2-hydroxyethyl)-1-piperazinyl]-3,7-dimethyl- (9CI) (CA INDEX NAME)

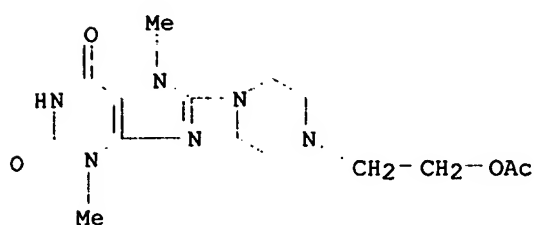


RN 67162-69-0 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-8-[4-(2-hydroxyethyl)-1-piperazinyl]-3,7-dimethyl-, monohydrobromide (9CI) (CA INDEX NAME)



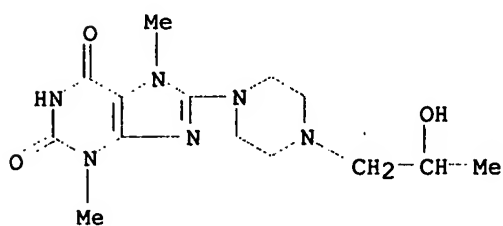
● HBr

RN 67162-70-3 CAPLUS
 CN 1H-Purine-2,6-dione, 8-[4-[2-(acetyloxy)ethyl]-1-piperazinyl]-3,7-dihydro-3,7-dimethyl-, monohydrobromide (9CI) (CA INDEX NAME)



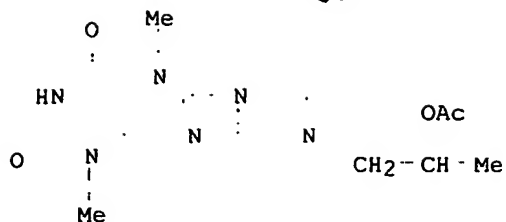
● HBr

RN 67162-72-5 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-8-[4-(2-hydroxypropyl)-1-piperazinyl]-3,7-dimethyl-, monohydrobromide (9CI) (CA INDEX NAME)

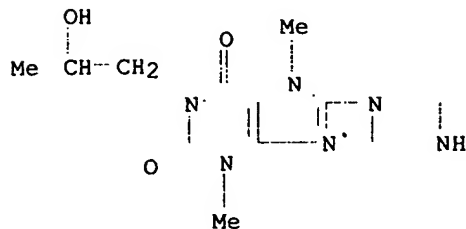


● HBr

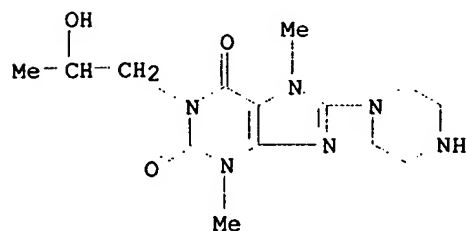
RN 67162-73-6 CAPLUS
 CN 1H-Purine-2,6-dione, 8-[4-[2-(acetyloxy)propyl]-1-piperazinyl]-3,7-dihydro-3,7-dimethyl- (9CI) (CA INDEX NAME)



RN 67162-74-7 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-1-(2-hydroxypropyl)-3,7-dimethyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)

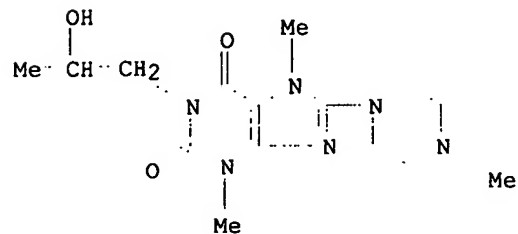


RN 67162-75-8 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-1-(2-hydroxypropyl)-3,7-dimethyl-8-(1-piperazinyl)-, dihydrobromide (9CI) (CA INDEX NAME)



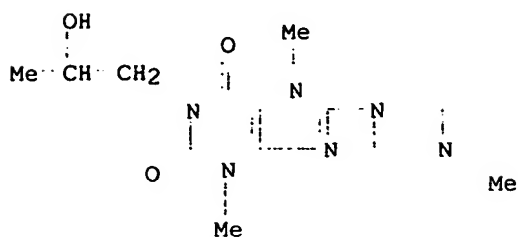
● 2 HBr.

RN 67162-76-9 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-1-(2-hydroxypropyl)-3,7-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



RN 67162-77-0 CAPLUS

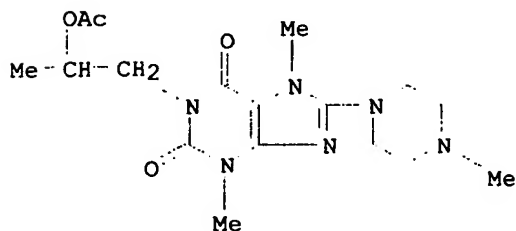
CN 1H-Purine-2,6-dione, 3,7-dihydro-1-(2-hydroxypropyl)-3,7-dimethyl-8-(4-methyl-1-piperazinyl)-, monohydrobromide (9CI) (CA INDEX NAME)



● HBr

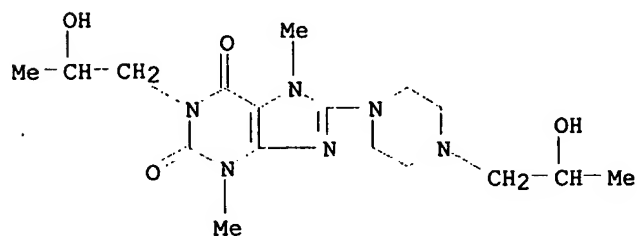
RN 67162-78-1 CAPLUS

CN 1H-Purine-2,6-dione, 1-[2-(acetyloxy)propyl]-3,7-dihydro-3,7-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



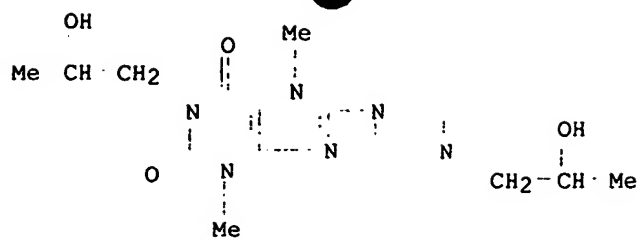
RN 67162-79-2 CAPLUS

CN 1H-Purine-2,6-dione, 3,7-dihydro-1-(2-hydroxypropyl)-8-[4-(2-hydroxypropyl)-1-piperazinyl]-3,7-dimethyl- (9CI) (CA INDEX NAME)



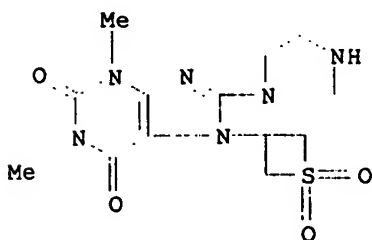
RN 67162-80-5 CAPLUS

CN 1H-Purine-2,6-dione, 3,7-dihydro-1-(2-hydroxypropyl)-8-[4-(2-hydroxypropyl)-1-piperazinyl]-3,7-dimethyl-, monohydrobromide (9CI) (CA INDEX NAME)

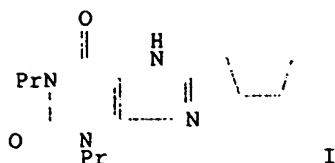


● HBr

AN 1998:260235 CAPLUS
 DN 129:49337
 TI Synthesis of biologically active derivatives of xanthine and benzimidazole
 AU Khaliullin, F. A.; Kataev, V. A.; Alekhin, E. K.; Volkova, S. S.; Nasyrov, Kh. M.; Strokin, Yu. V.
 CS Bashk. Gos. Med. Univ., Ufa, Russia
 SO Bashk. Khim. Zh. (1997), 4(4), 59-62
 CODEN: BKZHFU; ISSN: 0869-8406
 PB Izdatel'stvo "Reaktiv"
 DT Journal
 LA Russian
 CC 1-7 (Pharmacology)
 Section cross-reference(s): 28
 AB A study was done of reactions of amines with products of xanthines or benzimidazoles alkylation by epithiochlorohydrin. 2-Amino-substituted 1-(3-thietanyl)benzimidazoles were synthesized from 1-(3-thietanyl)-2-chlorobenzimidazole. 8-Amino-substituted derivs. were formed from 8-bromo-1,3-dimethyl-7-(1-oxothietanyl-3)- and 8-bromo-1,3-dimethyl-7-(1,1-dioxothietanyl-3)xanthines. 2-Amino-substituted 2,3-dihydrothiazolo[3.2-a]benzimidazoles were synthesized from 2-methylsulfonyl-1-(2,3-epithiopropyl)benzimidazole. Immunotropic and anti-inflammatory activities of the synthesized compds. were discovered.
 ST xanthine benzimidazole deriv epithiochlorohydrin prepn antiinflammatory
 IT Anti-inflammatory drugs
 Immunomodulators
 (prepn. of biol. active derivs. of xanthine and benzimidazole)
 IT 136265-52-6 208577-18-8 208577-19-9 208577-20-2
 RL: RCT (Reactant)
 (prepn. of biol. active derivs. of xanthine and benzimidazole)
 IT 51-17-2DP, Benzimidazole, derivs. 69-89-6DP, Xanthine, derivs.
 182193-10-8P 208577-04-2P 208577-05-3P 208577-06-4P 208577-07-5P
 208577-08-6P 208577-09-7P 208577-10-0P 208577-11-1P 208577-12-2P
 208577-13-3P 208577-14-4P 208577-15-5P 208577-16-6P
 208577-17-7P
 RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of biol. active derivs. of xanthine and benzimidazole)
 IT 208577-13-3P
 RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of biol. active derivs. of xanthine and benzimidazole)
 RN 208577-13-3 CAPLUS
 CN 1H-Purine-2,6-dione, 7-(1,1-dioxido-3-thietanyl)-3,7-dihydro-1,3-dimethyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)



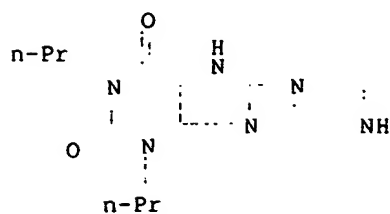
AN 1987:400259 CAPLUS
 DN 107:259
 TI Potent adenosine receptor antagonists that are selective for the A1
 receptor subtype
 AU Martinson, Elizabeth A.; Johnson, Roger A.; Wells, Jack N.
 CS Sch. Med., Vanderbilt Univ., Nashville, TN, 37232, USA
 SO Mol. Pharmacol. (1987), 31(3), 247-52
 CODEN: MOPMA3; ISSN: 0026-895X
 DT Journal
 LA English
 CC 1-3 (Pharmacology)
 GI



AB A systematic study of xanthine structure-activity relationships that compared antagonist potency at the A1 receptor of adipocytes with potency at the A2 receptor of platelets was conducted. Since adenosine receptors are coupled to adenylate cyclase in these tissues, inhibition of adenylate cyclase via A1 receptors and stimulation via A2 receptors were used as models of receptor activation. Antagonist potency was quantitated by Schild anal., which yields an est. of affinity (Ki) for the drug-receptor interaction. Ki Values of a series of xanthine analogs made it possible to identify structural modifications than enhanced antagonist selectivity for one receptor subtype over the other. Changes in the substituent at position 8 of the xanthine nucleus influenced antagonist potency at the A1 adenosine receptor more than at the A2 receptor. In particular, an 8-cyclohexyl or 8-cyclopentyl substituent promoted antagonist selectivity for the A1 receptor subtype. Thus, 1,3-dipropyl-8-cyclopentylxanthine (I) had comparatively high affinity (Ki = 0.47 nM) at the A1 receptor, and was roughly 150-fold more potent as an antagonist of the A1- than of the A2-adenosine receptor subtype. In addn., the cycloalkylxanthines were relatively ineffective as inhibitors of cyclic nucleotide phosphodiesterase when used at concns. that produce marked adenosine receptor antagonism.

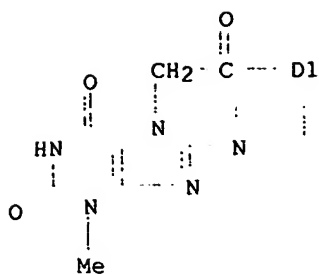
ST adenosine receptor antagonist structure activity
 IT Molecular structure-biological activity relationship
 (cyclic nucleotide phosphodiesterase-inhibiting, of xanthine derivs.)
 IT Neurotransmitter antagonists
 (purinergic A1, xanthine derivs. as)
 IT Molecular structure-biological activity relationship
 (purinergic A1 antagonist, of xanthine derivs.)
 IT 58-55-9, biological studies 69-89-6 69-89-6D, Xanthine, derivs.
 28822-58-4 31542-62-8 63908-26-9 63908-28-1 63908-29-2
 63908-30-5 63908-37-2 63908-39-4 72117-77-2 72117-80-7
 78033-12-2 78033-13-3 78033-15-5 85872-51-1 85872-53-3
 89073-57-4 102146-07-6 106686-66-2 108653-56-1 108653-57-2
 108653-58-3 108653-59-4 108653-60-7 108670-88-8
 RL: BIOL (Biological study)
 (A1- and A2-adenosine receptors antagonism by, structure in relation to)
 IT 9040-59-9, Cyclic nucleotide phosphodiesterase
 RL: PROC (Process)
 (inhibition of, by xanthine derivs., structure in relation to)
 IT 108653-58-3
 RL: BIOL (Biological study)
 (A1- and A2-adenosine receptors antagonism by, structure in relation to)
 RN 108653-58-3 CAPLUS

CN 1H-Purine-2,6-dione, 3,7-dihydro-8-(1-piperazinyl)-1,3-dipropyl- (9CI)
(CA INDEX NAME)

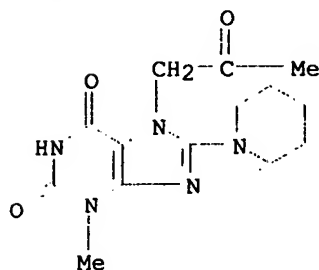


AN 1989:586916 CAPLUS
 DN 111:186916
 TI Properties and pharmacological action of derivatives of 7,8-disubstituted
 3-methylxanthine and 6H-8-methylimidazo[1,2-f]xanthine
 AU Skul'skaya, E. A.; Garmash, S. N.; Koval, N. B.; Priimenko, B. A.; Samura,
 B. A.
 CS Zaporozh. Med. Inst., Zaporozhe, USSR
 SO Farm. Zh. (Kiev) (1989), (4), 34-9
 CODEN: FRZKAP; ISSN: 0367-3057
 DT Journal
 LA Ukrainian
 CC 1-3 (Pharmacology)
 AB A group of 19 xanthine derivs. was prepd. by reactions of 7-acylalkyl
 derivs. of 8-bromo-3-methylxanthine with primary and secondary amines.
 The toxicity and pharmacol. properties of the resulting xanthines were
 studied and related to their mol. structure. Most of the compds. showed
 diuretic and psychotropic effects.
 ST xanthine deriv diuretic neurotropic structure prepn
 IT Toxicity
 (of xanthine derivs., structure in relation to)
 IT Diuretics
 Psychotropics
 (xanthine derivs. prepn. as, structure in relation to)
 IT Molecular structure-biological activity relationship
 (diuretic, of xanthine derivs.)
 IT Molecular structure-biological activity relationship
 (neurotropic, of xanthine derivs.)
 IT Molecular structure-biological activity relationship
 (toxic, of xanthine derivs.)
 IT 1076-22-8DP, 3-Methylxanthine, derivs. 123416-27-3P
 123496-36-6P 123496-37-7P 123496-38-8P 123496-39-9P
 123496-40-2P 123496-41-3P 123496-42-4P 123496-43-5P
 123496-44-6P 123496-45-7P 123496-46-8P 123496-47-9P 123496-48-0P
 123496-49-1P 123496-50-4P 123496-51-5P 123496-52-6DP, derivs.
 123496-53-7P 123519-05-1P 123519-06-2P
 RL: BAC (Biological activity or effector, except adverse); BPR (Biological
 process); SPN (Synthetic preparation); THU (Therapeutic use);
 BIOL (Biological study); PREP (Preparation); PROC (Process); USES
 (Uses)
 (prepn. and pharmacol. of, diuretic and neurotropic activity and
 structure in relation to)
 IT 90-04-0, (o-Methoxyphenyl)amine 95-53-4, reactions 106-40-1,
 (p-Bromophenyl)amine 106-49-0, (p-Methylphenyl)amine, reactions
 108-44-1, reactions 109-73-9, Butylamine, reactions 110-91-8,
 Morpholine, reactions 111-42-2, reactions 134-32-7, 1-Naphthalenamine
 150-75-4 617-89-0, 2-Furanmethanamine
 RL: RCT (Reactant)
 (reaction of, with bromomethylxanthines)
 IT 93703-24-3D, 8-Bromo-3-methylxanthine, acylalkyl derivs.
 RL: RCT (Reactant)
 (reaction of, with primary and secondary amines)
 IT 109-89-7, Diethylamine, reactions 110-89-4, Piperidine, reactions
 101072-01-9 101072-04-2 101072-05-3 101072-06-4 123416-26-2
 RL: RCT (Reactant)
 (reactions of, with primary and secondary amines)
 IT 123416-27-3P 123496-36-6P 123496-38-8P
 123496-42-4P 123496-43-5P 123519-05-1P
 RL: BAC (Biological activity or effector, except adverse); BPR (Biological
 process); SPN (Synthetic preparation); THU (Therapeutic use);
 BIOL (Biological study); PREP (Preparation); PROC (Process); USES
 (Uses)
 (prepn. and pharmacol. of, diuretic and neurotropic activity and
 structure in relation to)
 RN 123416-27-3 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-[2-oxo-2-(thienyl)ethyl]-8-(1-
 piperidinyl)- (9CI) (CA INDEX NAME)

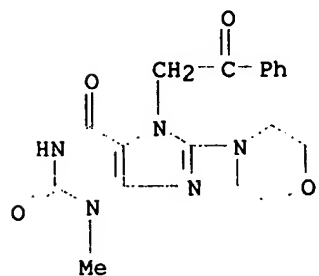
S



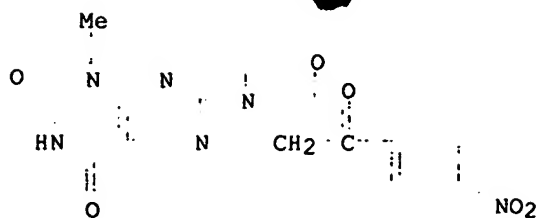
RN 123496-36-6 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-(2-oxopropyl)-8-(1-piperidinyl)- (9CI) (CA INDEX NAME)



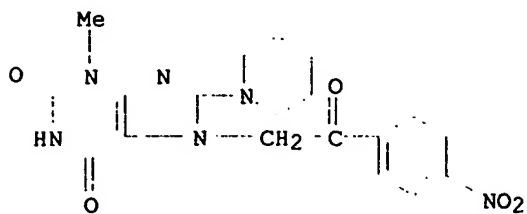
RN 123496-38-8 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-8-(4-morpholinyl)-7-(2-oxo-2-phenylethyl)- (9CI) (CA INDEX NAME)



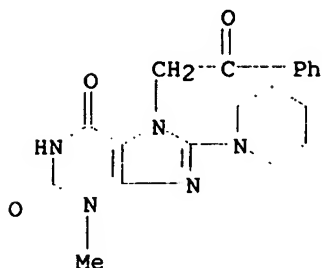
RN 123496-42-4 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-8-(4-morpholinyl)-7-[2-(4-nitrophenyl)-2-oxoethyl]- (9CI) (CA INDEX NAME)



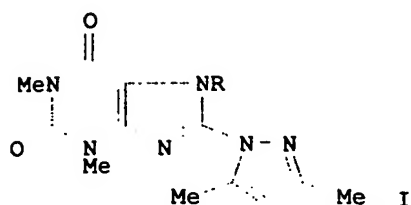
RN 123496-43-5 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-[2-(4-nitrophenyl)-2-oxoethyl]-8-(1-piperidinyl)- (9CI) (CA INDEX NAME)



RN 123519-05-1 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-(2-oxo-2-phenylethyl)-8-(1-piperidinyl)- (9CI) (CA INDEX NAME)

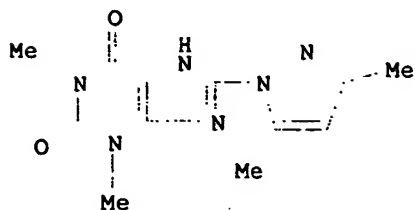


AN 1997:297890 CAPLUS
 DN 126:330513
 TI Synthesis and antiphlogistic effect of some 7-substituted
 8-(3,5-dimethyl-1-pyrazolyl) theophyllines
 AU Mazur, I. A.; Kremzer, O. A.; Korobko, D. B.; Samura, B. A.; Beljenkij, C.
 A.
 CS Kiev. Derzhavn. Med. Univ., Kiev, Ukraine
 SO Farm. Zh. (Kiev) (1996), (3), 82-84
 CODEN: FRZKAP; ISSN: 0367-3057
 PB Zdorov'ya
 DT Journal
 LA Ukrainian
 CC 26-9 (Biomolecules and Their Synthetic Analogs)
 Section cross-reference(s): 1
 OS CASREACT 126:330513
 GI

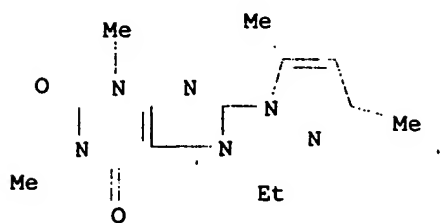


AB Fifteen title compds. I (R = H, alkyl, hydroxyalkyl, aryl), which showed
 effective antiinflammatory activity, were synthesized in 53.0-94.0% yield
 by cyclocondensation reaction of the corresponding 7-substituted
 8-hydrazinotheophyllines with (MeCO)2CH2 in refluxing glacial AcOH.
 ST pyrazolyl theophylline prepn antiinflammatory; cyclocondensation
 hydrazinotheophylline acetylacetone
 IT Anti-inflammatory drugs
 Cyclocondensation reaction
 (synthesis and antiinflammatory activity of some substituted
 (dimethylpyrazolyl)theophyllines by cyclocondensation of
 hydrazinotheophyllines with acetylacetone)
 IT 145351-66-2P 189689-48-3P 189689-49-4P
 189689-50-7P 189689-51-8P 189689-52-9P
 189689-53-0P 189689-54-1P 189689-55-2P
 189689-56-3P 189689-57-4P 189689-58-5P
 189689-59-6P 189689-60-9P 189689-61-0P
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic
 preparation); BIOL (Biological study); PREP (Preparation)
 (synthesis and antiinflammatory activity of some substituted
 (dimethylpyrazolyl)theophyllines by cyclocondensation of
 hydrazinotheophyllines with acetylacetone)
 IT 123-54-6, Acetylacetone, reactions 21266-25-1 78960-55-1 88552-69-6,
 8-Hydrazinotheophylline 113577-82-5 189689-62-1 189689-63-2
 189689-64-3 189689-65-4 189689-66-5 189689-67-6 189689-68-7
 189689-69-8 189689-70-1 189689-71-2 189689-72-3
 RL: RCT (Reactant)
 (synthesis and antiinflammatory activity of some substituted
 (dimethylpyrazolyl)theophyllines by cyclocondensation of
 hydrazinotheophyllines with acetylacetone)
 IT 145351-66-2P 189689-48-3P 189689-49-4P
 189689-50-7P 189689-51-8P 189689-52-9P
 189689-53-0P 189689-54-1P 189689-55-2P
 189689-56-3P 189689-57-4P 189689-58-5P
 189689-59-6P 189689-60-9P 189689-61-0P
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic
 preparation); BIOL (Biological study); PREP (Preparation)
 (synthesis and antiinflammatory activity of some substituted
 (dimethylpyrazolyl)theophyllines by cyclocondensation of

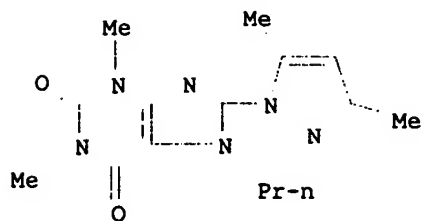
hydrazinotheophyllines with acetylacetone)
 RN 145351-66-2 CAPLUS
 CN 1H-Purine-2,6-dione, 8-(3,5-dimethyl-1H-pyrazol-1-yl)-3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



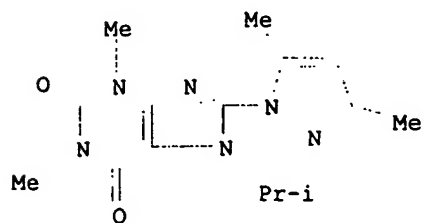
RN 189689-48-3 CAPLUS
 CN 1H-Purine-2,6-dione, 8-(3,5-dimethyl-1H-pyrazol-1-yl)-7-ethyl-3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



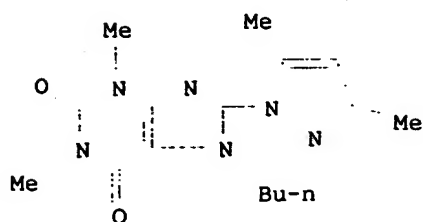
RN 189689-49-4 CAPLUS
 CN 1H-Purine-2,6-dione, 8-(3,5-dimethyl-1H-pyrazol-1-yl)-3,7-dihydro-1,3-dimethyl-7-propyl- (9CI) (CA INDEX NAME)



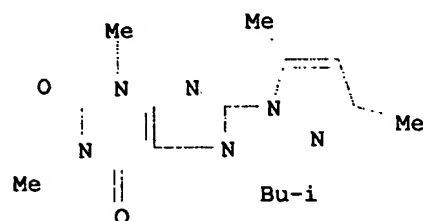
RN 189689-50-7 CAPLUS
 CN 1H-Purine-2,6-dione, 8-(3,5-dimethyl-1H-pyrazol-1-yl)-3,7-dihydro-1,3-dimethyl-7-(1-methylethyl)- (9CI) (CA INDEX NAME)



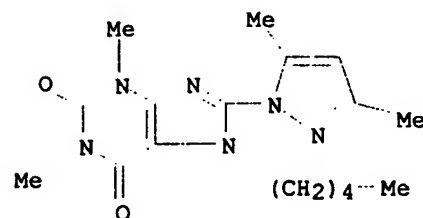
RN 189689-51-8 CAPLUS
 CN 1H-Purine-2,6-dione, 7-butyl-8-(3,5-dimethyl-1H-pyrazol-1-yl)-3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



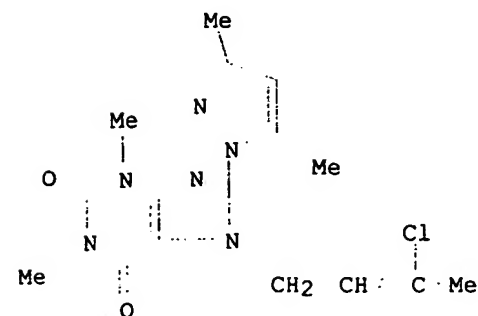
RN 189689-52-9 CAPLUS
 CN 1H-Purine-2,6-dione, 8-(3,5-dimethyl-1H-pyrazol-1-yl)-3,7-dihydro-1,3-dimethyl-7-(2-methylpropyl)- (9CI) (CA INDEX NAME)

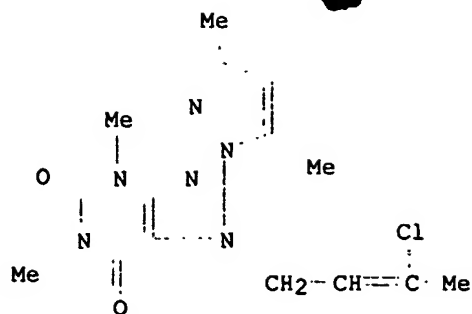


RN 189689-53-0 CAPLUS
 CN 1H-Purine-2,6-dione, 8-(3,5-dimethyl-1H-pyrazol-1-yl)-3,7-dihydro-1,3-dimethyl-7-pentyl- (9CI) (CA INDEX NAME)

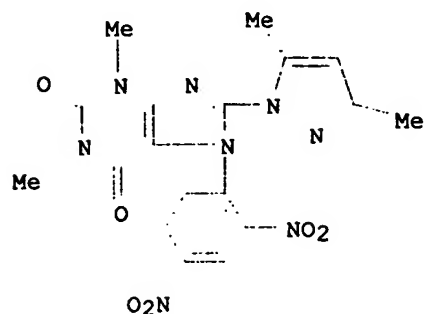


RN 189689-54-1 CAPLUS
 CN 1H-Purine-2,6-dione, 7-(3-chloro-2-butenyl)-8-(3,5-dimethyl-1H-pyrazol-1-yl)-3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)

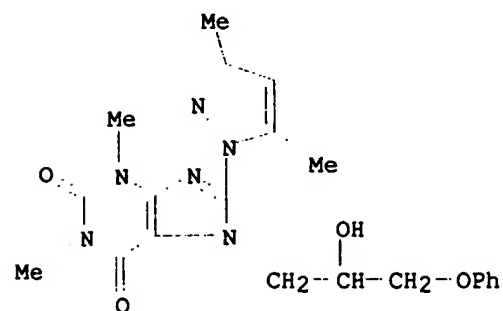




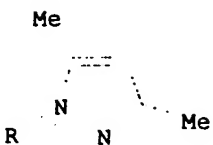
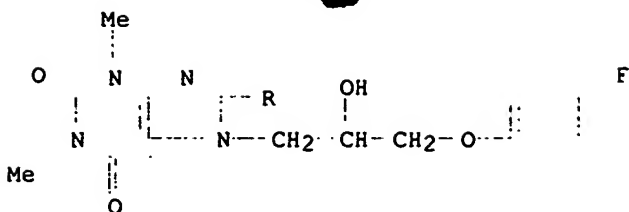
RN 189689-55-2 CAPLUS
 CN 1H-Purine-2,6-dione, 8-(3,5-dimethyl-1H-pyrazol-1-yl)-7-(2,4-dinitrophenyl)-3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



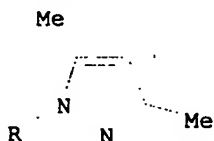
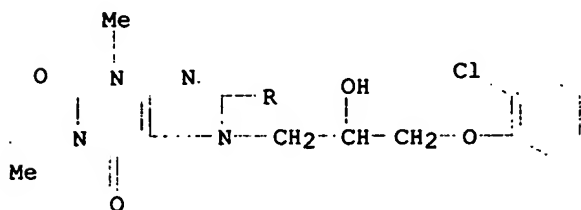
RN 189689-56-3 CAPLUS
 CN 1H-Purine-2,6-dione, 8-(3,5-dimethyl-1H-pyrazol-1-yl)-3,7-dihydro-7-(2-hydroxy-3-phenoxypropyl)-1,3-dimethyl- (9CI) (CA INDEX NAME)



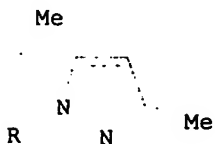
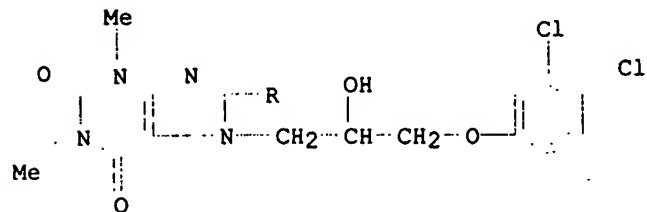
RN 189689-57-4 CAPLUS
 CN 1H-Purine-2,6-dione, 8-(3,5-dimethyl-1H-pyrazol-1-yl)-7-[3-(4-fluorophenoxy)-2-hydroxypropyl]-3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



RN 189689-58-5 CAPLUS
 CN 1H-Purine-2,6-dione, 7-[3-(2-chlorophenoxy)-2-hydroxypropyl]-8-(3,5-dimethyl-1H-pyrazol-1-yl)-3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)

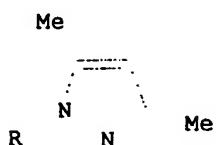
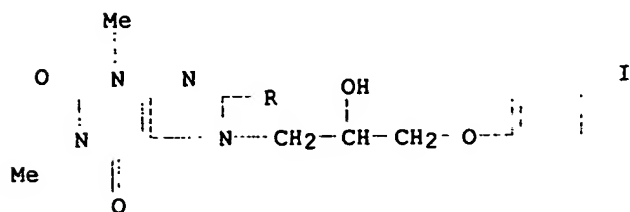


RN 189689-59-6 CAPLUS
 CN 1H-Purine-2,6-dione, 7-[3-(3,4-dichlorophenoxy)-2-hydroxypropyl]-8-(3,5-dimethyl-1H-pyrazol-1-yl)-3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



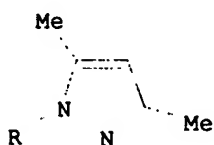
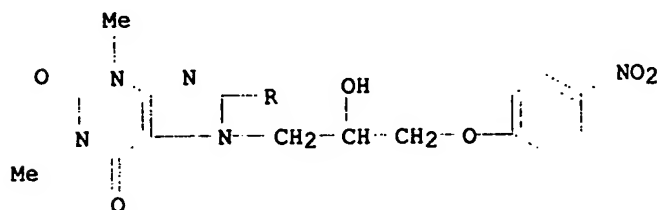
RN 189689-60-9 CAPLUS

CN 1H-Purine-2,6-dione, 8-(3,5-dimethyl-1H-pyrazol-1-yl)-3,7-dihydro-7-[2-hydroxy-3-(4-iodophenoxy)propyl]-1,3-dimethyl- (9CI) (CA INDEX NAME)

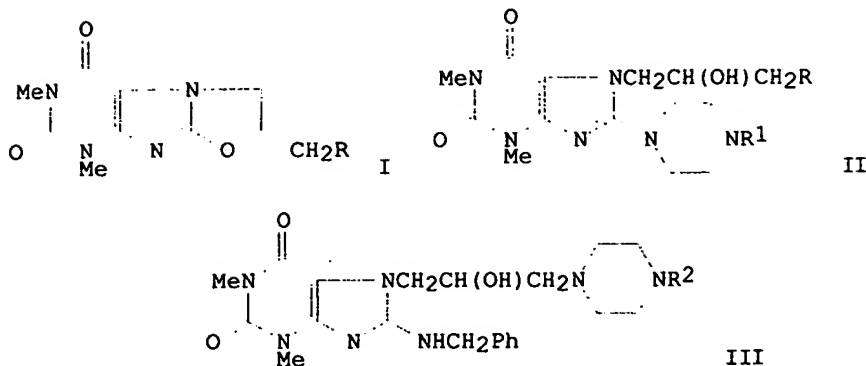


RN 189689-61-0 CAPLUS

CN 1H-Purine-2,6-dione, 8-(3,5-dimethyl-1H-pyrazol-1-yl)-3,7-dihydro-7-[2-hydroxy-3-(4-nitrophenoxy)propyl]-1,3-dimethyl- (9CI) (CA INDEX NAME)

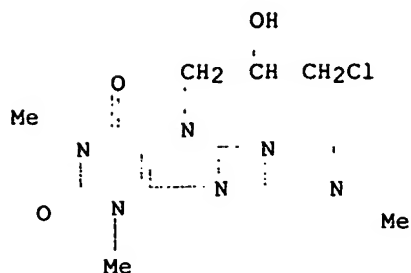


AN 1983:539617 CAPLUS
 DN 99:139617
 TI Synthesis and properties of 7- and 8-piperazinyl derivatives of theophylline
 AU Gorczyca, Maria; Pawlowski, Maciej; Lucka-Sobstel, Barbara
 CS Dep. Pharm. Chem., Sch. Med., Krakow, 31-065, Pol.
 SO Acta Pol. Pharm. (1982), 39(5-6), 315-21
 CODEN: APPHAX; ISSN: 0001-6837
 DT Journal
 LA Polish
 CC 26-9 (Biomolecules and Their Synthetic Analogs)
 Section cross-reference(s): 1
 GI



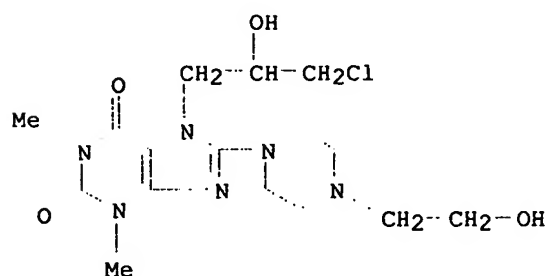
AB Aminolysis of the oxazole ring in I (R = H, Cl) with an N-substituted piperazine yielded II (R = H, Cl; R1 = Me, CH2CH2OH). II (R = Cl) were treated with an amine in the presence of KOH to give II (R = PhCH2NH, R1 = Me, CH2CH2OH; R = 4-methyl-1-piperazinyl, R1 = Me). An analogous reaction of I (R = Cl) with PhCH2NH2 followed by reaction with an N-substituted piperazine gave III (R2 = CH2CH2OH, CO2Et, Ph). II and III are potential cardiovascular agents.
 ST theophyllinylpropanolamine prepn cardiovascular;
 piperazinopropyltheophylline; piperazinotheophylline aminopropyl
 IT Cardiovascular agents
 (theophyllinylpropanolamines)
 IT 87080-28-2P 87080-29-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and amination of)
 IT 87080-30-6P 87080-31-7P 87080-32-8P 87080-33-9P
 87080-34-0P 87080-35-1P 87092-24-8P
 87092-25-9P 87092-26-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 IT 103-76-4 109-01-3
 RL: RCT (Reactant)
 (reaction of, with chloromethyloxazoxanthine)
 IT 92-54-6 100-46-9, reactions 103-49-1 120-43-4
 RL: RCT (Reactant)
 (reaction of, with chloropropyltheophyllines)
 IT 1021-74-5 25565-94-0 62932-78-9
 RL: RCT (Reactant)
 (reaction of, with piperazine derivs.)
 IT 87080-28-2P 87080-29-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and amination of)
 RN 87080-28-2 CAPLUS
 CN 1H-Purine-2,6-dione, 7-(3-chloro-2-hydroxypropyl)-3,7-dihydro-1,3-dimethyl-

8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



RN 87080-29-3 CAPLUS

CN 1H-Purine-2,6-dione, 7-(3-chloro-2-hydroxypropyl)-3,7-dihydro-8-[4-(2-hydroxyethyl)-1-piperazinyl]-1,3-dimethyl- (9CI) (CA INDEX NAME)



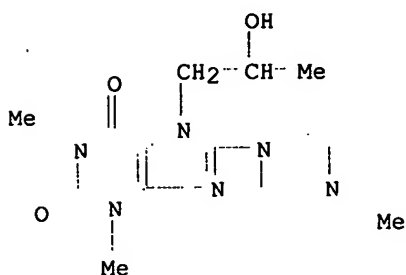
IT 87080-32-8P 87080-33-9P 87080-34-0P

87080-35-1P 87092-25-9P 87092-26-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

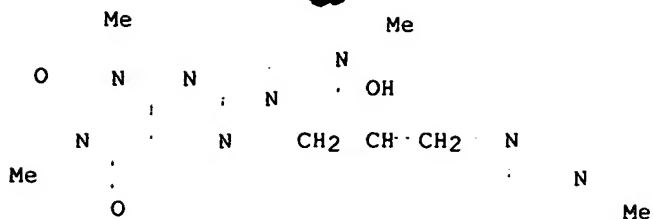
RN 87080-32-8 CAPLUS

CN 1H-Purine-2,6-dione, 3,7-dihydro-7-(2-hydroxypropyl)-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



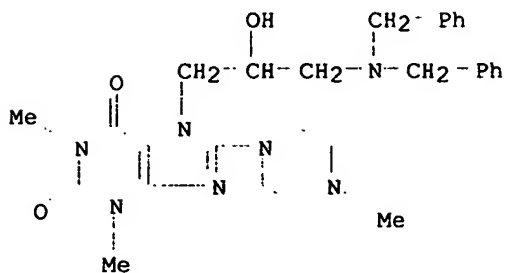
RN 87080-33-9 CAPLUS

CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-3-(4-methyl-1-piperazinyl)propyl]-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



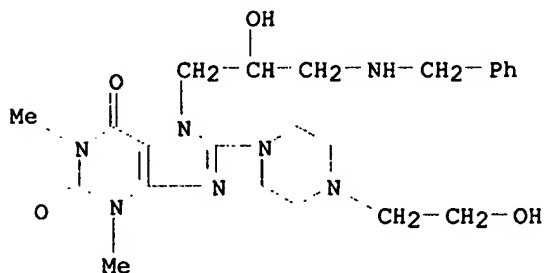
RN 87080-34-0 CAPLUS

CN 1H-Purine-2,6-dione, 7-[3-[(bis(phenylmethyl)amino)-2-hydroxypropyl]-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)]- (9CI) (CA INDEX NAME)



RN 87080-35-1 CAPLUS

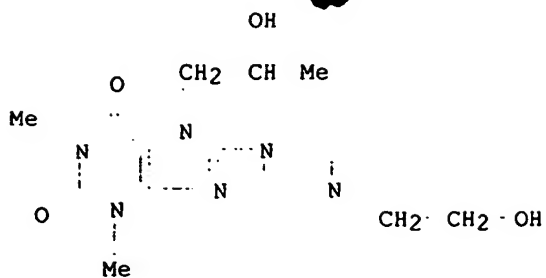
CN 1H-Purine-2,6-dione, 3,7-dihydro-8-[4-(2-hydroxyethyl)-1-piperazinyl]-7-[2-hydroxy-3-[(phenylmethyl)amino]propyl]-1,3-dimethyl-, dihydrochloride (9CI) (CA INDEX NAME)



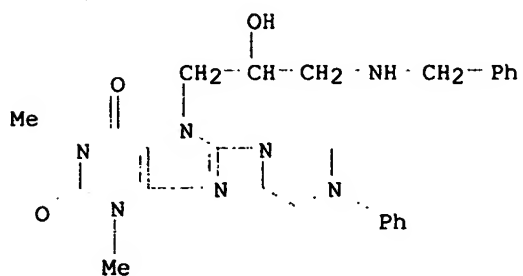
● 2 HCl

RN 87092-25-9 CAPLUS

CN 1H-Purine-2,6-dione, 3,7-dihydro-8-[4-(2-hydroxyethyl)-1-piperazinyl]-7-(2-hydroxypropyl)-1,3-dimethyl- (9CI) (CA INDEX NAME)



RN 87092-26-0 CAPLUS
 CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-3-
 [(phenylmethyl)amino]propyl]-1,3-dimethyl-8-(4-phenyl-1-piperazinyl)-,
 dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl